Preliminary analysis attempts to relate BCA surface area to the nitrogen cycle of ozone chemistry. Inclusion of the $HNO_3$ reaction with BCA in one model improves the agreement of calculated to measured $NO_x/NO_y$ ratios, but more work is yet to be done. The effect of the other reactions on the ratio needs to be explored. An assessment of the accuracy of the reaction probabilities should be made, if possible. Radiative effect must also be evaluated.

Katja Drdla of the National Research Council, Ross J. Salawitch of Jet Propulsion Laboratory, Sunita Verma of Science Systems and Applications Inc., and Steve Howard of Symtech collaborated with the investigators on this project.

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# Developing and Validating an Aerosol Model for the Upper Troposphere

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The main purpose of this research was to develop and validate an upper tropospheric aerosol model (UTAM). With this model it is possible to calculate the following quantities: (1) the equilibrium partitioning of various species between the gas and aqueous phases for a wide variety of environmental conditions, (2) the variation in the inorganic aerosol composition as a function of temperature and relative humidity, (3) the solution compositions at which inorganic salt precipitation might occur in upper tropospheric aerosols, and (4) the deliquescence relative humidity (in the atmosphere this is the ambient relative humidity at which a completely dry aerosol becomes thermodynamically unstable and will transform into an aqueous solution droplet) of ammoniated or nitrated aerosols under upper tropospheric conditions. Predicting the equilibrium partitioning has important applications in both gas- and aqueous-phase chemistry modeling calculations, and determining the aerosol composition and salt precipitation can play a significant role in predicting the frequency of cirrus cloud occurrence in the upper troposphere.

Currently, thermodynamic electrolyte models are available for calculating the properties of inorganic aerosols for the conditions found in the lower troposphere and stratosphere. In the lower troposphere, such models are often used in air-quality studies to assess the effects of aerosols on health, gas-phase partitioning, and visibility. In the stratosphere, aerosol models have been used to simulate the formation and growth of polar stratospheric clouds, which are linked to stratospheric ozone depletion. However, these thermodynamic treatments are not suited for calculating the properties of inorganic aerosols under upper tropospheric conditions. Since these aerosols participate in the nucleation and growth of cirrus clouds, understanding their physical properties is crucial for accurately predicting the occurrence of cirrus clouds in the upper troposphere and their subsequent radiative effects.

Simulating the thermodynamic properties of the upper-tropospheric aerosols would require a complex mixed-electrolyte model that accounts for the various ionic interactions in the aqueous solution. This project is developing a mixed-electrolyte model of upper-tropospheric aerosols to address in detail how the current model of cirrus formation from pure sulfuric acid solution droplets can be affected by the presence of ammonium or nitrate ions in solution. Basically, the research shows that ammoniated aerosols are more efficient in nucleating cirrus than are pure sulfuric acid droplets. Further, crude analysis of the recent Subsonic Aircraft: Contrail and Cloud Effects Special Study data indicates that most of the

aerosols collected during this campaign were composed of acidic solutions of ammonium sulfate instead of pure sulfuric acid, which is commonly used as the main source of cloud condensation nuclei for microphysical modeling of cirrus clouds in the upper troposphere. In general, it is essential to determine the phase of the background particles that exist in the upper troposphere since the barrier to ice cloud formation by vapor deposition on dry salt surfaces is significantly higher than that of homogeneous freezing from aqueous solution droplets. Also, detailed investigations of the role of aerosol composition and phase transformation in the nucleation and growth of cirrus clouds have been done. In the figure, the three main particle transport pathways to the upper troposphere are depicted and will be used to investigate how these various pathways may alter the nucleation of cirrus clouds in the upper troposphere.

Collaborators on this project were Jin S. Lin, Bay Area Environmental Research Institute and O. B. Toon, LASP Institute, University of Colorado, Boulder, Colorado.

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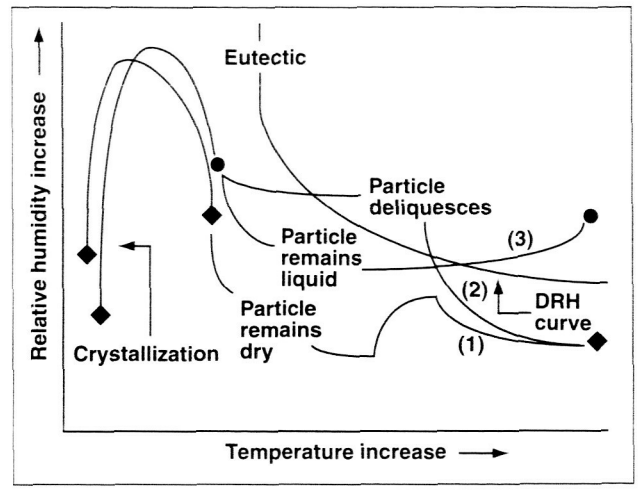


*Fig. 1. Particle transport pathways to the upper troposphere. Three general temperature-relative humidity pathways are shown in the plot. Dry and liquid particles are designated as diamonds and circles, respectively. Above the deliquescence relative humidity (DRH) curve the liquid particles are stable, and below this curve liquid particles become supercooled. Solid particles can only exist below the DRH curve for temperatures above the eutectic point.*